Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Elaidic acid (*trans*-9-octadecenoic acid)

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.102
wR factor = 0.256
Data-to-parameter ratio = 21.0

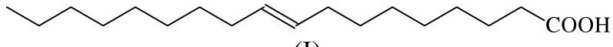
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 11 October 2005
Accepted 14 October 2005
Online 19 October 2005

Elaidic acid, $C_{18}H_{34}O_2$, has an essentially linear alkyl chain. The double bond is twisted across the mean direction of the alkyl chain in a skew′, *trans*, skew conformation. In the crystal structure, the molecules form centrosymmetric O—H···O hydrogen-bonded dimers (O···O = 2.684 Å).

Comment

The physical, biological and nutritional properties of fatty acids are largely determined by the number, position and configuration of their double bonds. These determine the shape of the molecules, the way molecules can pack together in solid phases, monolayers, bilayers *etc.*, and how individual molecules can interact with enzymes and receptors. Most natural unsaturated fatty acids have *cis* (*Z*) double bonds. Trans (*E*) fatty acids are present in dairy fats and are produced during the catalytic partial hydrogenation used in the production of hardened fats and during deodorization of commodity oils. The labelling of foods with *trans* content is increasingly required due to their undesirable nutritional properties. Alternative ways of producing hardened fats, such as interesterification or blending with fully saturated fats, and milder deodorization procedures, are being developed to reduce *trans* content. Trans fatty acids more closely resemble saturated acids in melting point and nutritional properties, sharing an essentially linear structure which allows closely aligned packing in condensed phases. In contrast, *cis* double bonds introduce a bend in the alkyl chain, making packing less stable and lowering the melting point. We have determined the structure of elaidic acid (*trans*-9-octadecenoic acid), (I), to enable a detailed comparison of a *trans* fatty acid with saturated and *cis*-unsaturated compounds.



(I)

Relatively few crystal structures of fatty acids are available, as good crystals are difficult to obtain, often being thin plates and often crystallizing in several polymorphs. Most monoenes have low melting points and polyenes are liquids at room temperature. The crystal structures of the following saturated and monoene C_{18} fatty acids have been reported to date: stearic acid (octadecanoic acid) (Malta *et al.*, 1971; Kaneko *et al.*, 1990, 1994*a*,*b*), oleic acid (*cis*-9-octadecenoic acid) (Abrahamsson & Ryderstedt-Nahringbauer, 1962; Kaneko *et al.*, 1997) and petroselinic acid (*cis*-6-octadecenoic acid) (Kaneko *et al.*, 1992*a*,*b*). No *trans*-octadecenoic acid structure has been reported to date.

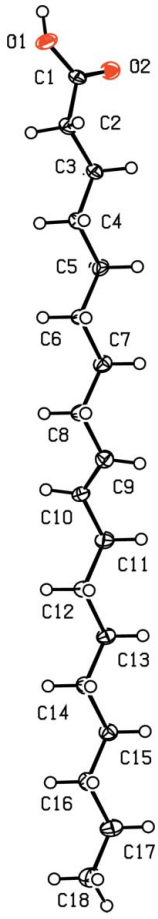


Figure 1
A view of (I), with displacement ellipsoids drawn at the 30% probability level.

Elaidic acid (I) has an essentially linear alkyl chain, with the torsion angle between saturated C atoms close to 180° (Table 1). The C7—C8—C9—C10, C8—C9—C10—C11 and C9—C10—C11—C12 torsion angles are −118.8 (4), −179.9 (4) and 118.6 (4)°, respectively, resulting in the double bond being twisted across the mean direction of the alkyl chain in a skew′, *trans*, skew conformation. The C1–C18 distance is 21.393 (6) Å, comparable with that in fully extended stearic acid structures (21.6 Å; Malta *et al.*, 1971; Kaneko *et al.*, 1990, 1994*b*). This contrasts with the *cis*-octadecenoic acids, where the molecules are bent and the C1–C18 distance is reduced to between 17.8 and 19.7 Å (Abrahamsson & Ryderstedt-Nahringbauer, 1962; Kaneko *et al.*, 1997, 1992*a*,*b*).

In the crystal structure of (I), molecules related by inversion centres are linked by O—H···O hydrogen bonds to form $R_2^2(8)$ dimers (Bernstein *et al.*, 1995) typical of carboxylic acids (Table 2).

Experimental

A commercial sample of (I) (Sigma, Poole, Dorset, UK) was recrystallized from ethanol at room temperature. The crystals were composed of very thin stacked sheets which tended to be twisted. After many attempts, a crystal was found from which it was possible to obtain a data set.

Crystal data

$C_{18}H_{34}O_2$
M_r = 282.45
Monoclinic, $C2/c$
a = 98.48 (2) Å
b = 4.9381 (3) Å
c = 7.1826 (8) Å
β = 92.570 (12)°
V = 3489.4 (8) Å^3
Z = 8
D_x = 1.075 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3830 reflections
θ = 3.3–27.6°
μ = 0.07 mm^{-1}
T = 120 (2) K
Plate, colourless
0.20 × 0.18 × 0.01 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.987, T_{max} = 0.999
17532 measured reflections
3830 independent reflections
1679 reflections with $I > 2\sigma(I)$
R_{int} = 0.150
θ_{max} = 27.6°
$h = -126 \rightarrow 126$
$k = -6 \rightarrow 6$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.102
$wR(F^2)$ = 0.256
S = 1.08
3830 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0744P)^2 + 7.8445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected torsion angles (°).

C1—C2—C3—C4	−170.7 (3)	C9—C10—C11—C12	118.6 (4)
C2—C3—C4—C5	177.0 (3)	C10—C11—C12—C13	178.4 (3)
C3—C4—C5—C6	−176.6 (3)	C11—C12—C13—C14	−179.8 (3)
C4—C5—C6—C7	178.9 (3)	C12—C13—C14—C15	179.9 (3)
C5—C6—C7—C8	−179.1 (3)	C13—C14—C15—C16	179.8 (3)
C6—C7—C8—C9	−178.4 (3)	C14—C15—C16—C17	−179.6 (3)
C7—C8—C9—C10	−118.8 (4)	C15—C16—C17—C18	179.5 (3)
C8—C9—C10—C11	−179.9 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.87	1.86	2.684 (3)	158

Symmetry code: (i) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$.

H atoms were treated as riding, with C—H(aromatic) = 0.95 and C—H(CH$_2$) = 0.99 Å, with U_{iso}(H) = 1.2U_{eq}(C), *C*—*H*(methyl) = 0.98 Å, with U_{iso}(H) = 1.5U_{eq}(C), and O—H = 0.87 Å, with U_{iso}(H) = 1.5U_{eq}(O). The O-bound H atom was allowed to ride at its position as determined from a difference map. Although the best crystal was selected from many crystallization attempts, the higher than usual values for R, wR and R_{int} may be a result of the crystal quality. The possibilty that the crystal was twinned was investigated but this did not give any significant results.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

The X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. The Scottish Crop Research Institute receives grant-in-aid from the Scottish Executive Environmental and Rural Affairs Department.

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supporting information

Acta Cryst. (2005). E**61**, o3730–o3732 [https://doi.org/10.1107/S1600536805033040]

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trans-9-octadecenoic acid

Crystal data

$C_{18}H_{34}O_2$
$M_r = 282.45$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 98.48$ (2) Å
$b = 4.9381$ (3) Å
$c = 7.1826$ (8) Å
$\beta = 92.570$ (12)°
$V = 3489.4$ (8) Å^3
$Z = 8$
$F(000) = 1264$
$D_x = 1.075$ Mg m^{-3}
Melting point: 318 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3830 reflections
$\theta = 3.3$–27.6°
$\mu = 0.07$ mm^{-1}
$T = 120$ K
Plate, colourless
0.20 × 0.18 × 0.01 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker Nonius FR91 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.987$, $T_{max} = 0.999$
17532 measured reflections
3830 independent reflections
1679 reflections with $I > 2\sigma(I)$
$R_{int} = 0.150$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.3°$
$h = -126 \rightarrow 126$
$k = -6 \rightarrow 6$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.102$
$wR(F^2) = 0.256$
$S = 1.08$
3830 reflections
182 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0744P)^2 + 7.8445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

Experimental. The scale factors in the experimental table are calculated from the 'size' command in the *SHELXL97* input file.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.73264 (3)	0.7933 (8)	0.6134 (6)	0.0228 (10)
O1	0.74261 (2)	0.9565 (6)	0.6713 (4)	0.0309 (8)
O2	0.73386 (2)	0.6167 (6)	0.4964 (4)	0.0248 (7)
C2	0.71969 (3)	0.8502 (8)	0.7109 (5)	0.0201 (10)
C3	0.70703 (3)	0.7093 (8)	0.6268 (6)	0.0205 (10)
C4	0.69400 (3)	0.8111 (8)	0.7115 (5)	0.0189 (9)
C5	0.68092 (3)	0.6865 (8)	0.6249 (6)	0.0209 (10)
C6	0.66795 (3)	0.8041 (8)	0.7042 (6)	0.0192 (9)
C7	0.65479 (3)	0.6840 (8)	0.6155 (6)	0.0217 (10)
C8	0.64192 (3)	0.8070 (8)	0.6941 (6)	0.0217 (10)
C9	0.62897 (3)	0.6835 (8)	0.6108 (5)	0.0228 (10)
C10	0.61931 (3)	0.8140 (8)	0.5146 (5)	0.0218 (10)
C11	0.60645 (3)	0.6909 (8)	0.4322 (6)	0.0245 (10)
C12	0.59348 (3)	0.8106 (8)	0.5097 (5)	0.0193 (9)
C13	0.58035 (3)	0.6919 (8)	0.4225 (6)	0.0218 (10)
C14	0.56738 (3)	0.8113 (8)	0.4988 (6)	0.0208 (10)
C15	0.55429 (3)	0.6890 (8)	0.4087 (6)	0.0223 (10)
C16	0.54127 (3)	0.8076 (8)	0.4853 (6)	0.0224 (10)
C17	0.52827 (3)	0.6812 (9)	0.3945 (6)	0.0282 (11)
C18	0.51520 (3)	0.7981 (9)	0.4725 (7)	0.0360 (12)
H1	0.7506	0.9756	0.6267	0.046*
H2A	0.7181	1.0481	0.7094	0.024*
H2B	0.7210	0.7940	0.8428	0.024*
H3A	0.7079	0.5117	0.6478	0.025*
H3B	0.7065	0.7411	0.4906	0.025*
H4A	0.6935	1.0102	0.6969	0.023*
H4B	0.6945	0.7711	0.8467	0.023*
H5A	0.6811	0.4884	0.6464	0.025*
H5B	0.6807	0.7170	0.4885	0.025*
H6A	0.6679	1.0026	0.6849	0.023*
H6B	0.6681	0.7704	0.8402	0.023*
H7A	0.6546	0.7151	0.4793	0.026*
H7B	0.6548	0.4860	0.6367	0.026*
H8A	0.6422	0.7806	0.8309	0.026*
H8B	0.6418	1.0043	0.6697	0.026*
H9	0.6277	0.4949	0.6294	0.027*
H10	0.6206	1.0025	0.4956	0.026*
H11A	0.6066	0.4935	0.4565	0.029*
H11B	0.6062	0.7173	0.2955	0.029*
H12A	0.5936	0.7795	0.6459	0.023*
H12B	0.5935	1.0088	0.4888	0.023*
H13A	0.5804	0.4938	0.4437	0.026*
H13B	0.5802	0.7224	0.2862	0.026*
H14A	0.5673	1.0094	0.4776	0.025*
H14B	0.5675	0.7802	0.6350	0.025*

H15A	0.5542	0.7206	0.2725	0.027*
H15B	0.5544	0.4908	0.4295	0.027*
H16A	0.5411	1.0055	0.4635	0.027*
H16B	0.5414	0.7770	0.6216	0.027*
H17A	0.5282	0.7132	0.2583	0.034*
H17B	0.5285	0.4830	0.4152	0.034*
H18A	0.5151	0.7603	0.6063	0.054*
H18B	0.5073	0.7141	0.4086	0.054*
H18C	0.5149	0.9943	0.4521	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0142 (16)	0.022 (2)	0.032 (3)	0.0038 (16)	−0.0035 (17)	0.005 (2)
O1	0.0171 (11)	0.0333 (19)	0.042 (2)	−0.0079 (12)	0.0022 (12)	−0.0123 (15)
O2	0.0219 (12)	0.0276 (18)	0.0251 (18)	−0.0011 (12)	0.0008 (11)	−0.0047 (15)
C2	0.0194 (16)	0.022 (2)	0.019 (3)	0.0035 (16)	−0.0021 (15)	−0.0017 (19)
C3	0.0166 (16)	0.020 (2)	0.025 (3)	0.0031 (15)	−0.0015 (16)	0.0035 (19)
C4	0.0191 (16)	0.019 (2)	0.019 (2)	0.0016 (15)	0.0015 (16)	−0.0005 (18)
C5	0.0183 (16)	0.019 (2)	0.025 (3)	−0.0030 (16)	−0.0059 (16)	0.0025 (19)
C6	0.0163 (16)	0.021 (2)	0.020 (3)	−0.0015 (15)	0.0024 (15)	0.0008 (19)
C7	0.0201 (16)	0.025 (2)	0.020 (3)	−0.0024 (16)	−0.0050 (16)	0.0019 (19)
C8	0.0194 (17)	0.028 (2)	0.018 (3)	−0.0018 (16)	0.0021 (16)	0.0018 (19)
C9	0.0232 (17)	0.024 (3)	0.022 (3)	−0.0005 (17)	0.0028 (17)	−0.001 (2)
C10	0.0154 (16)	0.023 (2)	0.026 (3)	−0.0026 (16)	0.0004 (16)	0.001 (2)
C11	0.0197 (17)	0.026 (2)	0.027 (3)	−0.0010 (16)	−0.0068 (17)	0.001 (2)
C12	0.0187 (16)	0.025 (2)	0.014 (2)	0.0003 (16)	−0.0002 (15)	0.0013 (19)
C13	0.0193 (17)	0.026 (2)	0.020 (3)	−0.0018 (16)	−0.0023 (16)	0.0005 (19)
C14	0.0209 (17)	0.021 (2)	0.020 (3)	0.0010 (16)	−0.0022 (16)	0.0010 (19)
C15	0.0205 (17)	0.025 (2)	0.021 (3)	0.0001 (16)	−0.0032 (16)	−0.002 (2)
C16	0.0232 (17)	0.021 (2)	0.023 (3)	0.0019 (16)	−0.0003 (17)	−0.0014 (19)
C17	0.0207 (17)	0.037 (3)	0.027 (3)	−0.0025 (17)	−0.0039 (17)	0.001 (2)
C18	0.0263 (19)	0.040 (3)	0.041 (3)	−0.0003 (19)	−0.0041 (19)	0.002 (2)

Geometric parameters (Å, º)

C1—O2	1.221 (5)	C10—C11	1.502 (4)
C1—O1	1.323 (4)	C10—H10	0.95
C1—C2	1.508 (5)	C11—C12	1.535 (5)
O1—H1	0.8642	C11—H11A	0.99
C2—C3	1.528 (4)	C11—H11B	0.99
C2—H2A	0.99	C12—C13	1.527 (4)
C2—H2B	0.99	C12—H12A	0.99
C3—C4	1.530 (5)	C12—H12B	0.99
C3—H3A	0.99	C13—C14	1.530 (5)
C3—H3B	0.99	C13—H13A	0.99
C4—C5	1.534 (4)	C13—H13B	0.99
C4—H4A	0.99	C14—C15	1.540 (4)

C4—H4B	0.99	C14—H14A	0.99
C5—C6	1.536 (5)	C14—H14B	0.99
C5—H5A	0.99	C15—C16	1.534 (5)
C5—H5B	0.99	C15—H15A	0.99
C6—C7	1.537 (4)	C15—H15B	0.99
C6—H6A	0.99	C16—C17	1.542 (4)
C6—H6B	0.99	C16—H16A	0.99
C7—C8	1.536 (5)	C16—H16B	0.99
C7—H7A	0.99	C17—C18	1.540 (5)
C7—H7B	0.99	C17—H17A	0.99
C8—C9	1.512 (4)	C17—H17B	0.99
C8—H8A	0.99	C18—H18A	0.98
C8—H8B	0.99	C18—H18B	0.98
C9—C10	1.318 (5)	C18—H18C	0.98
C9—H9	0.95		

O2—C1—O1	123.9 (3)	C9—C10—H10	117.1
O2—C1—C2	124.3 (3)	C11—C10—H10	117.1
O1—C1—C2	111.8 (4)	C10—C11—C12	113.7 (3)
C1—O1—H1	128.4	C10—C11—H11A	108.8
C1—C2—C3	115.1 (3)	C12—C11—H11A	108.8
C1—C2—H2A	108.5	C10—C11—H11B	108.8
C3—C2—H2A	108.5	C12—C11—H11B	108.8
C1—C2—H2B	108.5	H11A—C11—H11B	107.7
C3—C2—H2B	108.5	C13—C12—C11	114.0 (3)
H2A—C2—H2B	107.5	C13—C12—H12A	108.8
C2—C3—C4	112.2 (3)	C11—C12—H12A	108.8
C2—C3—H3A	109.2	C13—C12—H12B	108.8
C4—C3—H3A	109.2	C11—C12—H12B	108.8
C2—C3—H3B	109.2	H12A—C12—H12B	107.7
C4—C3—H3B	109.2	C12—C13—C14	114.2 (3)
H3A—C3—H3B	107.9	C12—C13—H13A	108.7
C3—C4—C5	114.3 (3)	C14—C13—H13A	108.7
C3—C4—H4A	108.7	C12—C13—H13B	108.7
C5—C4—H4A	108.7	C14—C13—H13B	108.7
C3—C4—H4B	108.7	H13A—C13—H13B	107.6
C5—C4—H4B	108.7	C13—C14—C15	113.3 (3)
H4A—C4—H4B	107.6	C13—C14—H14A	108.9
C4—C5—C6	113.3 (3)	C15—C14—H14A	108.9
C4—C5—H5A	108.9	C13—C14—H14B	108.9
C6—C5—H5A	108.9	C15—C14—H14B	108.9
C4—C5—H5B	108.9	H14A—C14—H14B	107.7
C6—C5—H5B	108.9	C16—C15—C14	113.4 (3)
H5A—C5—H5B	107.7	C16—C15—H15A	108.9
C5—C6—C7	113.6 (3)	C14—C15—H15A	108.9
C5—C6—H6A	108.8	C16—C15—H15B	108.9
C7—C6—H6A	108.8	C14—C15—H15B	108.9
C5—C6—H6B	108.8	H15A—C15—H15B	107.7

C7—C6—H6B	108.8	C15—C16—C17	112.6 (3)
H6A—C6—H6B	107.7	C15—C16—H16A	109.1
C8—C7—C6	112.9 (3)	C17—C16—H16A	109.1
C8—C7—H7A	109.0	C15—C16—H16B	109.1
C6—C7—H7A	109.0	C17—C16—H16B	109.1
C8—C7—H7B	109.0	H16A—C16—H16B	107.8
C6—C7—H7B	109.0	C18—C17—C16	112.7 (3)
H7A—C7—H7B	107.8	C18—C17—H17A	109.0
C9—C8—C7	113.0 (3)	C16—C17—H17A	109.0
C9—C8—H8A	109.0	C18—C17—H17B	109.0
C7—C8—H8A	109.0	C16—C17—H17B	109.0
C9—C8—H8B	109.0	H17A—C17—H17B	107.8
C7—C8—H8B	109.0	C17—C18—H18A	109.5
H8A—C8—H8B	107.8	C17—C18—H18B	109.5
C10—C9—C8	125.9 (4)	H18A—C18—H18B	109.5
C10—C9—H9	117.1	C17—C18—H18C	109.5
C8—C9—H9	117.1	H18A—C18—H18C	109.5
C9—C10—C11	125.7 (4)	H18B—C18—H18C	109.5

O2—C1—C2—C3	−11.8 (6)	C8—C9—C10—C11	−179.9 (4)
O1—C1—C2—C3	168.8 (3)	C9—C10—C11—C12	118.6 (4)
C1—C2—C3—C4	−170.7 (3)	C10—C11—C12—C13	178.4 (3)
C2—C3—C4—C5	177.0 (3)	C11—C12—C13—C14	−179.8 (3)
C3—C4—C5—C6	−176.6 (3)	C12—C13—C14—C15	179.9 (3)
C4—C5—C6—C7	178.9 (3)	C13—C14—C15—C16	179.8 (3)
C5—C6—C7—C8	−179.1 (3)	C14—C15—C16—C17	−179.6 (3)
C6—C7—C8—C9	−178.4 (3)	C15—C16—C17—C18	179.5 (3)
C7—C8—C9—C10	−118.8 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.87	1.86	2.684 (3)	158

Symmetry code: (i) −*x*+3/2, −*y*+3/2, −*z*+1.